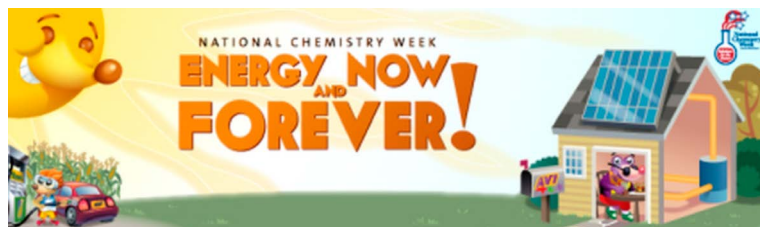


# The Crucible

www.pittsburghacs.org

Volume: XCIX No.2

October 2013



**YOU ARE INVITED!!!**

**Join the Pittsburgh Section ACS as We Celebrate  
National Chemistry Week!**

**Where: Carnegie Science Center  
When: October 25-26, 2013**

The 2013 National Chemistry Week (NCW) celebrations in Pittsburgh will be held on Friday, October 25 (10 AM to 3 PM) and Saturday, October 27 (10 AM to 5 PM), at the Carnegie Science Center.

Join in the NCW activities as we celebrate this year's NCW theme  
*"Energy: Now and Forever!"*

- Hands-on Activities - Theater Shows – Prizes
- Visit over 20 tables with hands-on experiments, activities, and demonstrations
- Visit the Drake Oil Well Museum's Mobile Energy Education Training Unit, located in the Carnegie Science Center's parking lot, on Friday, October 25
- Catch special NCW-related theater shows
- Register to win a chemistry set or one of several prizes

For more information about the NCW celebration in Pittsburgh, visit the Pittsburgh Section ACS's website at [www.pittsburghacs.org/outreach/national-chemistry-week/](http://www.pittsburghacs.org/outreach/national-chemistry-week/)

**Find us on Facebook at: Pittsburgh ACS NCW**

You can also contact the Carnegie Science Center at (412) 237-1640 or the Pittsburgh Section ACS's NCW Coordinator Michael Mautino at (412) 777-4792 / [michael.mautino@bayer.com](mailto:michael.mautino@bayer.com)

The Pittsburgh Section's 2013 NCW activities are sponsored by the Society for Analytical Chemists of Pittsburgh, the Spectroscopy Society of Pittsburgh, the PPG Industries Foundation, the PPG Science Education Council, the Carnegie Science Center, and Bayer Corporation.

## Pittsburgh Section Wins ChemLuminary Awards

The Pittsburgh Section ACS was awarded two prestigious ChemLuminary Awards in Indianapolis on September 10, 2013. The awards were for the Environmental Group and their best Sustainability Program and for Outstanding Large Local Section for 2012.

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## October Meeting

Monday, October 7, 2013

8:00 PM

Duquesne University

### *“Raman Microspectroscopy and Advanced Statistics for Forensic Applications”*

**Igor Lednev, Ph.D.**

University at Albany, State University of New York

**Abstract:** The identification of biological stains recovered at a crime scene is a key part of forensic investigation. Biochemical presumptive and confirmatory tests are destructive, require hazardous and expensive reagents and/or suffer from cross-reactivity with other biological fluids. Each of these problems has significant negative impacts on efficiency, cost, lead-time, and quality of the forensic investigation. There is no a single test which can be used for several body fluids. We have demonstrated that Raman microspectroscopy combined with advanced statistics has a great potential as easy-to-use, automatic, on-field method for rapid, nondestructive, confirmatory identification of body fluid traces at a crime scene. We have developed a Raman spectroscopic library for identification of all major body fluids including blood, semen, saliva, vaginal fluid and sweat. In addition, the ability of the method to differentiate between animal and human blood traces, as well as between venous and menstrual blood has been shown. The method has been expanded to body fluid mixtures, contaminated traces and stains on various substrates. Preliminary exciting results on the genetic profiling based on Raman signature of blood and semen will be also discussed.

Near-infrared (NIR) Raman microspectroscopy and attenuated total reflectance (ATR) Fourier transform infrared spectroscopy (FTIR) combined with advanced statistics was also utilized for detection, characterization and identification of gunshot residue (GSR). The firearm discharge process is analogous to a complex chemical reaction. The reagents of this process are represented by the chemical composition of the ammunition, firearm and cartridge case. The specific firearm parameters determine the conditions of the reaction and thus the subsequent product, GSR. We found that Raman and IR spectra collected from these products are characteristic for different caliber ammunition. This study demonstrates for the first time that vibrational spectroscopy has the potential for the differentiation of GSR based upon forensically relevant parameters, such as caliber size.

A new concept of multidimensional spectroscopic signature and adequate software have been introduced and developed to take into account the intrinsic sample heterogeneity. This concept improves the identification and differentiation power of the method and could be applied for a variety of practical problems involving heterogeneous sample.

**Biography:** Dr. Igor K. Lednev is an associate professor at the University at Albany, State University of New York. He graduated from the Moscow Institute of Physics and Technology, Russian Federation, receiving his Ph.D. degree in

**Continued on page 13**

**Dinner Reservations:** Please email the SACP Administrative Assistant, Valarie Daugherty at [daugherty@pittcon.org](mailto:daugherty@pittcon.org) by Tuesday October 1, 2013 to make dinner reservations. Should you not have email, please call 412-825-3220, ext 204. Dinner will cost \$8 (\$4 for students) and checks are to be made out to the SACP. If you have any dietary restrictions, please let Valarie know when you leave a message.

**Parking:** Duquesne University Parking Garage entrance is on Forbes Avenue. Upon entering the garage, you will need to get a parking ticket and drive to upper floors. Bring your parking ticket to the dinner or meeting for a validation sticker. Please contact Duquesne University, if any difficulties should arise.

## ACS Energy Technology Group

Tuesday, October 8, 2013

*“Water Management In Unconventional Gas Industry:  
What We Know And What We Need To Find Out?”*

**Professor Radisav Vidic**  
**University of Pittsburgh**

**Social Hour 6:00 PM, Dinner 6:30 PM, Talk 7:30 PM**

**Spaghetti Warehouse**  
**26<sup>th</sup> & Smallman Streets, Strip District, Pittsburgh PA**  
**Free parking behind the restaurant**

Natural gas from unconventional sources has been gaining in its overall share of the energy market in the US and in the world. The Marcellus Shale is a geologic formation located approximately 7,000 ft. below the surface in parts of Pennsylvania (almost 70 percent of Pennsylvania sits atop the Marcellus Shale formation), West Virginia and New York, which is estimated to contain up to 500 trillion cubic feet of natural gas with about \$500 billion worth of recoverable gas. Gas recovery from deep shale formations like the Marcellus was historically far too costly until recent advances in horizontal drilling and multi-stage hydraulic fracturing created means of accessing these deposits. These state-of-the-art drilling methods use millions of gallons of water and have the potential to generate millions of gallons of polluted water. The movement of this water as well as the recovery and transmission of the produced natural gas has the potential to cause significant environmental disruption through multiple effects; including water withdrawals, wastewater disposal, air toxin releases, truck traffic, and noise pollution. These technical and environmental issues must be understood and properly addressed in order to fully utilize all the benefits of this energy resource. This presentation will address water management alternatives, their environmental implications, and future research needs.

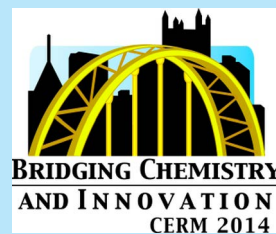
Radisav D. Vidic, Ph.D., P.E., is William Kepler Whiteford Professor of Environmental Engineering and Chairman of the Department of Civil and Environmental Engineering at the Swanson School of Engineering, University of Pittsburgh. Dr. Vidic holds a BS in Civil Engineering from the University of Belgrade (1987) and received his graduate education in Civil and Environmental Engineering from the University of Illinois (M.S., 1989) and University of Cincinnati (Ph.D., 1992). His research efforts focus on advancing the applications of surface science by providing fundamental understanding of molecular-level interactions at interfaces, water management for Marcellus shale development, and reuse of impaired waters for cooling systems in coal-fired power plants. Dr. Vidic has published over 250 journal papers and conference proceedings on these topics. He was elected by the Pittsburgh section of American Society of Civil Engineers as 2008 Professor of the Year and received the 2013 AEESP University Research Grand Prize for Excellence in Environmental Engineering and Science.

**For reservations, please contact Elliott Bergman at [elliott.acstechnology@gmail.com](mailto:elliott.acstechnology@gmail.com) by 1:00 on October 7<sup>th</sup>. Walk-ins are welcome. Our meetings are open to all. Cash or check payable to: Energy Tech Pgh Section ACS.**

The cost of the dinner is \$20 including tax and gratuity. Alcoholic drinks cost extra. Please specify your preference from the following menu choices: Spaghetti with meatballs, 15-layer lasagna, Four-cheese manicotti, Fettuccini Alfredo, Pesto Pasta, or Grilled chicken Caesar salad. Please indicate special needs such as vegetarian, gluten-free, etc.

## CERM 2014 Call for Technical Session Topics and Organizers

The 45<sup>th</sup> Central Regional Meeting of the American Chemical Society is being held in Pittsburgh October 1-4, 2014. The Program Committee will be soliciting suggestions for Session Topics and Organizers through NOVEMBER 1, 2013. You can access a link to submit your topics on our website: [www.pittsburghACS.org](http://www.pittsburghACS.org). Any questions regarding Programming should be directed to Program Co-Chairs Dr. Adrian Michael ([amichael@pitt.edu](mailto:amichael@pitt.edu)) or Dr. Michelle Ward ([muscat@pitt.edu](mailto:muscat@pitt.edu)).



## CERM 2014 Save the Date!

The Central Regional Meeting of the ACS will be held October 1-4, 2014 at the Doubletree by Hilton Green Tree Hotel, Pittsburgh.

For more information, visit the CERM website at [www.acscerm2014.org](http://www.acscerm2014.org).

Presents

**ACS "ON THE ROAD" MEETING  
MILDRED PERRY MEMORIAL LECTURE****Tuesday, October 8, 2013*****"Aqueous Electrolyte Polyionic Electrochemical  
Cells For Scaled Stationary Energy Storage"*****Speaker:**

Dr. Jay F. Whitacre

Founder and CTO - Aquion Energy



This presentation will cover the conception, scaling, and implementation of energy storage electrochemical batteries intended for stationary storage applications. These devices use heretofore unexplored electrode interactions that exploit multi-cation reactions that occur simultaneously at different degrees depending on cell state of charge. The core device uses a configuration wherein the active anode material consists of a blend of  $\text{NaTi}_2(\text{PO}_4)_3$  and activated carbon and the cathode is cubic spinel  $\lambda\text{-MnO}_2$  that has resident lithium. The electrolyte is a blend of  $\text{Li}^+$  and  $\text{Na}^+$  and hydrogen (at some states of charge) cation species, with  $\text{SO}_4^-$  and  $\text{OH}^-$  (at some states of charge) as the countering anions, solvated in a neutral pH aqueous electrolyte. The basic function of the battery will be discussed, and comparisons between small bench top cells and fully scaled product-level devices will be drawn. Data will be presented showing that large scale industrially packaged batteries with nearly 3000 Wh in capacity have been produced and qualified. Further data will show that packs of these batteries in the multi-kWh range have been effectively implemented in field-testing around the world. These applications include support for both smaller off-grid applications with bus voltages in the in the 20 to 100 V range, as well as, grid compatible systems with bus voltages in excess of 1000 V.

Key topics include: a description of the core electrochemical technology; a description of the path to scaled production of these devices; lifetime performance of this system through a range of temperatures; data from field tests in relevant applications showing the performance of our batteries under application specific load profiles; and a vision for future implementation of this technology on a massive scale.

**Schedule of Events**

5:00	Swanson Science Center Tour/Student Research Posters
6:00	ACS Regional Meeting – Swanson Science Center Atrium
6:15	Dinner – Rossin Campus Center Ballroom
7:15	Speaker Presentation – Dieter-Porter Lecture Hall

**Dinner Reservations:** A sit-down dinner (chicken entrée) will cost \$15 for members and \$5 for students. Checks can be made out to Washington and Jefferson College and mailed to Patricia Brletic (ATTN: Science on the Road) at 60 S. Lincoln Street, Washington, PA 15301. Please make dietary restrictions known when you RSVP. For dinner reservations, please call Patricia Brletic at 724-223-6130 or email her at [pbrletic@washjeff.edu](mailto:pbrletic@washjeff.edu) by 1:00 PM, October 4, 2013.

**Directions:** Please see the Pittsburgh Section website [www.pittsburghacs.org](http://www.pittsburghacs.org) for directions to the event.



## Pittsburgh Section ACS Younger Chemists Committee

Thank you for your support for our 2013 YCC Chemistry Carnival! For October we will host an interactive and informative event for the local section.

The ACS Younger Chemists Committee has teamed up with ACS Webinars and ACS Careers to bring you a “**Program-in-a-box**” called ***Putting Your Best Foot Forward: Managing Your Paper and Online Resumes*** on October 8. Dave Harwell from ACS Careers will be giving a presentation followed by a panel discussion with chemistry recruiters. You will have access to:

- Expert speakers with a **LIVE** question and answer session.
- Brochures and flyers from ACS Career Services on job search resources and how to access free career consultants.
- Discussion questions and talking points for after the webinar.
- ACS Webinars beaker mugs that we will raffle off as a door prize.

Please visit our webpage [pghycc.org](http://pghycc.org) to learn more about the program and to sign in for this event. We hope to see you on October 8<sup>th</sup>.

### **What?**

*Putting Your Best Foot Forward: Managing  
Your Paper and Online Resumes*

### **Where?**

University of Pittsburgh  
(check our website [pghycc.org](http://pghycc.org) for the classroom number)

### **When?**

Tuesday, October 8, 2013  
7:00 PM - 8:00 PM EDT

## Pittsburgh Section ACS Members Receive Awards and Honors

Congratulations to the following Pittsburgh Section ACS Members.

### ***Terrence J. Collins - 2013 ACS Fellow***

Dr. Terry Collins from Carnegie Mellon University was one of only 96 ACS Fellows named in 2013. This honor is bestowed upon members for their outstanding accomplishments in scientific research, education, and public service.

### ***Dr. Kris Matyjaszewski - Madison Marshall Award***

Dr. Kris Matyjaszewski from Carnegie Mellon University is the winner of the Madison Marshall Award from the ACS North Alabama Section. The award recognizes an outstanding research chemist who has brought international distinction to himself and to the chemical profession.

### ***Dr. Peter Wipf - Morley Medal***

Dr. Peter Wipf from the University of Pittsburgh is the winner of the Morley Medal from the Cleveland Section. The award recognizes significant contributions to chemistry through achievements in research, teaching, engineering, research administration, and public service, outstanding service to humanity, or industrial progress in the region.



## Join the Greater Pittsburgh Area Women Chemists Committee in raising funds for Breast Cancer Awareness...

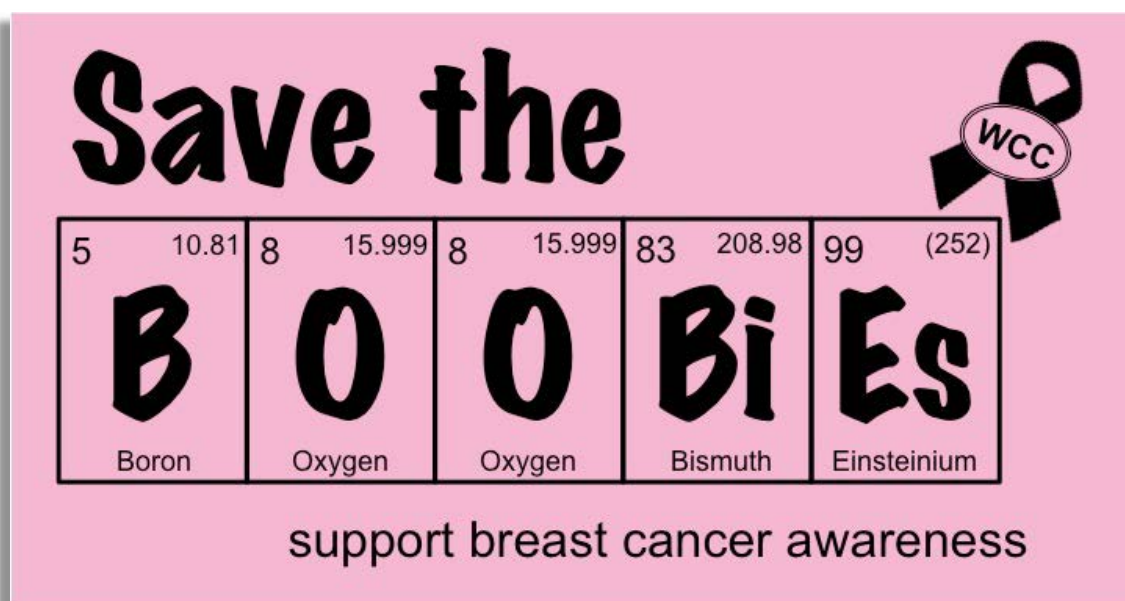
The WCC will be holding several fundraisers again this year to raise money for the *Young Women's Breast Cancer Awareness Foundation* at Magee Hospital.

Last year we donated \$1200 and we want to top that this year!

The first is a t-shirt sale, where all net proceeds will be donated.

The t-shirts will have the logo shown below and cost \$10/shirt.

*Preorders are due October 2<sup>nd</sup>!*



Please make check payable to *WCC* and mail along with this order form to:  
Dr. Michelle Ward / Room 107 / 219 Parkman Avenue / Pittsburgh, PA 15260.

You can also use the online form and PayPal link available on our website ([www.pitt.edu/~pghwcc](http://www.pitt.edu/~pghwcc)).  
(You will be contacted when shirts are ready for pick-up.)

Name: \_\_\_\_\_

Email: \_\_\_\_\_ Phone: \_\_\_\_\_

# small: \_\_\_\_\_ # x-large: \_\_\_\_\_

# medium: \_\_\_\_\_ # 2XL: \_\_\_\_\_

# large: \_\_\_\_\_ total enclosed: \$ \_\_\_\_\_

Spectroscopy Society of Pittsburgh presents:

# Laboratory Tour

of the

# University of Pittsburgh Structural Biology Facility

**Date:** Saturday, October 12, 2013  
**Time:** 930AM – 1 PM (free lunch included)  
**Location:** University of Pittsburgh  
Biomedical Science Tower 3 (3501 Fifth Ave Pgh 15213)

Agenda: 9:30 am Registration open (Biomedical Science Tower 3, 1st floor, along the Fifth avenue)  
10:00 am Introduction of Structural Biology  
10:30 am Facility Tour  
X-ray  
Electron Microscope  
Nuclear Magnetic Resonance  
Noon Lunch and Short seminars for Structural Biology Methods  
1:15 pm Discussion and networking  
1:45 pm Closing

Teachers Act48 may be available upon request (check to Rieko Ishima)

- Registration MUST be completed in advance
- Registration Fee is \$10.00 per person
- Photo Identification REQUIRED for entrance
- Registration to SSP members and one guest (full name and agency affiliation of guest required)
- Participants must be at least 18 years of age
- Tour of the Magnet facility is prohibited for those participants with a heart pacemaker or electronic equivalent
- Parking available at: Forbes-Semple Garage (check parking needed box on registration)  
Public Parking along Forbes Avenue (check parking NOT needed box on registration)

To register, complete the form below, and send it and a registration fee(s) to Ms. Shana Tokarski, c/o SSP, 300 Penn Center Blvd., Suite 332, Pittsburgh, PA 15235, no later than October 1, 2013. Checks can be made payable to SSP. Registration is limited to 30 participants.

Name \_\_\_\_\_ Phone No. \_\_\_\_\_

Agency \_\_\_\_\_ E-mail address \_\_\_\_\_

Guest Name \_\_\_\_\_ Agency \_\_\_\_\_

PARKING (select one)  Parking needed  Parking NOT needed

BOXED LUNCH (select one)  Vegetable & Cheese  Chicken  NO LUNCH



# The Spectroscopy Society of Pittsburgh



## October Meeting

Wednesday, October 16, 2013

Duquesne University – Bayer Learning Center (Wolfe Lecture Hall)

Technology Forum Speaker's Presentation 5:30 PM

Social Hour 5:30 PM • Dinner in the City View Café (6th Floor) 6:30 PM

Business Meeting 8:00 PM • Technical Program Speaker's Presentation 8:15 PM

### TECHNICAL PROGRAM - 8:15 PM

#### *"The Mars Curiosity Rover: A Year of Exploration and Evidence of Habitable Environments Beyond Earth"*

Professor Ralph Milliken, Brown University

**Abstract:** NASA's Curiosity rover has been exploring the red planet for the past year and has made a number of amazing discoveries. From flowing streams to muddy lake beds, the ancient rocks that have been examined so far have revealed that Mars was possibly much more hospitable to life several billions of years ago than previously imagined. The Curiosity rover is truly a laboratory on wheels and its payload is comprised of the most technically sophisticated instruments ever flown to Mars, allowing for these discoveries to be made. In addition to numerous cameras that measure light at visible and near-infrared wavelengths, the rover also utilizes laser induced breakdown spectroscopy, X-ray diffraction, alpha particle X-ray spectroscopy, and gas chromatograph mass spectroscopy. This presentation will describe the scope of the mission, what the rover team has learned over the past year by using these instruments, and what we expect in the coming months as Curiosity approaches its ultimate goal, the >3 mile tall Mt. Sharp.

**Bio:** Dr. Ralph Milliken, currently Assistant Professor of Geological Sciences at Brown University, received his B.S. in Geology from Indiana University and M.S./Ph.D. in Geology from Brown University (2006). After receiving his doctorate, he spent four years at NASA's Jet Propulsion Lab and the California Institute of Technology as a postdoctoral researcher and research scientist, where he first became involved in the Mars Science Laboratory rover project. Dr. Milliken joined the faculty in the Dept. of Civil Engineering and Geological Sciences at the University of Notre Dame in 2010 and then the faculty at Brown in 2012. His research interests include reflectance and emittance spectroscopy as applied to natural materials and linking lab, field, and airborne/satellite data to address geological problems. Studies focus on quantitative modeling of reflectance spectra, the formation, stability, and behavior of hydrous minerals, and, at a broader scale, the use of remote sensing techniques for determining the composition and geologic history of planetary bodies. In his spare time, Dr. Milliken enjoys music and spending time outdoors with his family.

### TECHNOLOGY FORUM - 5:30 PM

#### *"Potentially Hazardous Objects: Earth's Great Equalizer"*

Robert Marshall, Program Development Coordinator, Buhl Planetarium & Observatory at Carnegie Science Center

On February 15 of this year, Russian citizens of Chelyabinsk were surprised when a meteor blew up in the atmosphere, 14 miles high, injuring over one thousand people-the exact day astronomers were monitoring a 150ft near-Earth asteroid pass under geosynchronous satellites. How did we know about the one, but not the other? There are trillions of comets and asteroids orbiting our sun, but how do scientists determine which of these are near or on a collision course with Earth? More importantly, which of these should worry humankind if large enough to cause the destruction of a city, or worse? Learn what NASA researchers are uncovering about these relics of our solar system and the future engineering humanity must invest in if we are to protect ourselves from the inevitable.

**Bio** Robert J. Marshall is a graduate of the University of Pittsburgh with a B.S. in the field of astronomy, math, and the natural sciences. As program development coordinator and educator for the Buhl Planetarium and Observatory, he is employed at Carnegie Science Center where he presents real astronomical data to the public, develops curriculum for both University of Pittsburgh and Carnegie Mellon Osher programs, and travels the country for Fisher Science Education inspiring the teaching community. Furthermore, Robert has participated in research at Allegheny Observatory and is currently participating with NASA research through the Infrared Processing and Analysis Center (IPAC) home to the Spitzer Space Telescope.

**Dinner Reservations:** Please register on-line at <http://www.ssp-pgh.org/monthly-meeting-rsvp/> to make dinner reservations NO LATER THAN FRIDAY, October 11, 2013. Dinner will cost \$8 and checks can be made out to the SSP. If you have any dietary restrictions, please indicate them when you RSVP. **Parking Instructions:** The Duquesne University Parking Garage is located on Forbes Avenue. Upon entering the garage, receive parking ticket and drive to upper floors. Pick up a parking chit at the dinner or meeting.





# The Society for Analytical Chemists of Pittsburgh



Presents a Continuing Education Symposium

## Supernatural Seminar

Saturday, October 19, 2013

Chevron Science Center (Room 150)  
219 Parkman Avenue - Pittsburgh, PA 15260

9:00 – 9:30	Registration
9:30 – 10:00	Patty Wilson (Historian, Author)
10:00 – 10:30	Scott Crownover (Technical Equipment Specialist)
10:30 – 10:50	Q & A
11:00 - 12:00	Hayden Thomas - Haunted Pittsburgh Tours (Virtual Tour)
12:00 – 1:00	Lunch

### Registration Deadline: October 11, 2013

Registration Fee: \$10 (Lunch and Parking at Soldiers and Sailors Included), \$5 for students and retirees

Please make check payable to SACP and mail the registration form below to:

Valerie Daugherty  
SACP – Continuing Education Symposium  
300 Penn Center Boulevard, Suite 332  
Pittsburgh, PA 15235

REGISTRATION IS LIMITED TO THE FIRST 50 PEOPLE. GUESTS INCLUDING CHILDREN ARE WELCOME.

Everyone loves a good ghost story because of the unexplained occurrences, eerie noises, and spooky figures that all occur in macabre nightmarish settings. On October 19<sup>th</sup> learn more about the science of parapsychology.

Name: \_\_\_\_\_ Affiliation: \_\_\_\_\_

Mailing Address: \_\_\_\_\_

Email: \_\_\_\_\_ Phone: \_\_\_\_\_

Please note any dietary restrictions.

I am not staying for lunch.

I will need a parking pass.

# National Chemistry Week

## 2013 Illustrated Poem Contest:

### “Energy: Now and Forever!”

The Pittsburgh Section of the American Chemical Society (ACS) is sponsoring an illustrated poem contest for students in Kindergarten - 12th grade.

Contest Deadline: **Entries must be received at the address below by Friday, October 25, 2013.**

Prizes: **\$50 1st place and \$25 2nd place in each of 4 grade categories: K-2nd, 3rd-5th, 6th-8th and 9th-12th grades.**

**Mail entries to: Michael Mautino, 3485 Frye Ave, Finleyville, PA 15332. On back of entry include student name, grade, school name, teacher name, teacher phone number, and teacher e-mail address.**

Winners of the Pittsburgh illustrated poem contest will advance to the ACS National Illustrated Poem Contest!

Write and illustrate a poem using the NCW theme, **“Energy: Now and Forever!”**. Your poem must be **no more** than 40 words, and in the following styles to be considered:

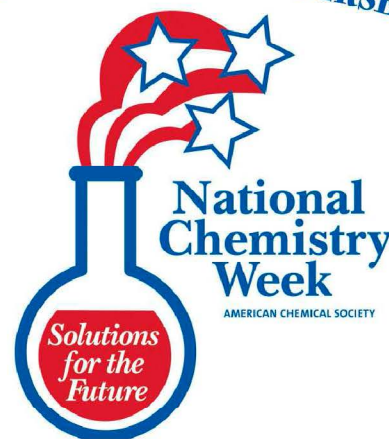
**HAIKU • LIMERICK • ODE • ABC POEM • FREE VERSE • END RHYME • BLANK VERSE**

**Participants are encouraged to explore topics related to:**

- Sustainable energy
- Chemical change into energy
- Sources of power
- Any other relevant topics

**Entries will be judged based upon:**

- Relevance to and incorporation of the theme
- Adherence to poem style
- Word choice and imagery
- Originality and creativity
- Colorful artwork
- Overall presentation



**Contest Rules:**

- Poems must conform to a particular style. No poem may be longer than 40 words.
- The topic of the poem and the illustration must be related to the NCW 2013 theme, **“Energy: Now and Forever!”**.
- All entries must be original works without aid from others.
- Each poem must be submitted and illustrated on an unlined sheet of paper (of any type) not larger than 11” x 14”. The illustration must be created by hand using crayons, watercolors, other types of paint,

colored pencils or markers. The text of the poem should be easy to read and may be printed with a computer, before the hand-drawn illustration is added, or the poem may be written on lined paper which is cut out and pasted onto the unlined paper with the illustration.

- Only one entry per student will be accepted.
- All illustrated poems and/or digital representations of the poems become the property of the American Chemical Society.
- Acceptance of prizes constitutes consent to use winners' names, likenesses and entries for editorial, advertising and publicity purposes.



# Society for Analytical Chemists of Pittsburgh



**November Meeting**  
**Monday, November 4, 2013**  
**8:00 PM**  
**Duquesne University**

***“In-Vivo Solid Phase Microextraction”***

**Janusz Pawliszyn, Ph.D.**  
Department of Chemistry, University of Waterloo

**Abstract:** In recent years, there has been a lot of interest in monitoring levels of biologically active compounds in living systems in their natural environments. These efforts are a significant departure from conventional ‘sampling’ techniques, where a portion of the system under study is removed from its natural environment, and the compounds of interest extracted and analyzed in a laboratory environment. There are two main motivations for exploring these types of investigations. The first one is the desire to study chemical processes in association with the normal biochemical milieu of a living system, and the second one is the lack of availability or impracticality of removing suitable samples from a living system, frequently because of size.

In the presentation I will describe the use of solid-phase microextraction (SPME) for in vivo sampling of drugs and metabolites in the tissue of freely moving animals that eliminates the need for tissue withdrawal in order to obtain quantitative analytical information. In comparison to the established in-vivo technique of microdialysis, in vivo SPME provides the advantages of reduced matrix effect, improved spatial resolution, better compatibility with LC-MS due to minimization of ionization suppression effects, improved extraction of unstable species and hydrophobic compounds. In contrast, in vivo microdialysis provides better temporal resolution resulting in semi-continuous monitoring in almost real-time. I will also describe the initial results of the collaborative research with Toronto General Hospital focused on development of low invasive tool for monitoring organ function during transplantation. Monitoring of the graft function before transplantation, especially by screening the profile of entire metabolome can provide important information to the physicians and therefore help in making decision of clinical matter. However, this type of analysis requires collecting tissue sample followed by its homogenization and solvent extraction. Such a procedure is not convenient and not recommended because of its high invasiveness, particularly when it needs to be repeated for monitoring purpose. In the current studies we used pig model to demonstrate the use of SPME for in situ extraction from organs in living donors, grafts undergo standard and experimental preservation methods as well as from the organs after transplantation and reperfusion.

**Biography:** Janusz Pawliszyn is a Professor and Canada Research Chair at the University of Waterloo. Dr. Pawliszyn received his B.Sc./Chem.Eng. in 1977 and M.Sc. in 1978 at Technical University of Gdansk; Ph.D. in 1982 at Southern Illinois University; PDF. in 1984 at University of Toronto.

Professor Pawliszyn has supervised 41 PhD and 62 MS students and he is an author of over 450 scientific publications and a book on Solid Phase Microextraction. His Hirsch Index (H-index) is 75. He is a Fellow of Royal Society of Canada and Chemical Institute of Canada, editor of *Analytica Chimica Acta*, *Trends in Analytical Chemistry* and a member of the Editorial Board of *Journal of Separation Science* and *Journal of Pharmaceutical Analysis*. He initiated a conference, “ExTech”, focusing on new advances in sample preparation and disseminates new scientific developments in the area, which meets every year in different part of the world. He received the 1995 McBryde Medal, the 1996 Tswett Medal, the 1996 Hyphenated Techniques in Chromatography Award, the 1996 Caledon Award, the

**Continued on Page 13**

**Dinner Reservations:** Please email the SACP Administrative Assistant, Valarie Daugherty at [daugherty@pittcon.org](mailto:daugherty@pittcon.org) by Tuesday, October 29, 2013 to make dinner reservations. Should you not have email, please call 412-825-3220, ext. 204. Dinner will cost \$8 (\$4 for students) and checks are to be made out to the SACP. If you have any dietary restrictions, please let Valarie know when you leave a message.

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# University of Pittsburgh Department of Chemistry

## Fall Lecture Series

### October 9, 2013

33<sup>rd</sup> Annual  
Pittsburgh Conference Lectures  
4:00pm  
150 Chevron  
Dr. Paul Alivisatos  
University of California - Berkeley  
*"Nanoscience and the Future of the Global Carbon Cycle"*

### October 10, 2013

33<sup>rd</sup> Annual  
Pittsburgh Conference Lectures  
2:30pm  
150 Chevron  
Dr. Paul Alivisatos  
University of California - Berkeley  
*"Design and Synthesis of Multi-Component Colloidal Nanocrystals for Catalysis and Sensing"*

### October 17, 2013

2:30pm  
150 Chevron  
Dr. Michael Pollastri  
Northeastern University  
*"Target Repurposing Accelerates Drug Discovery for Neglected Tropical Diseases"*

4:00pm  
150 Chevron

Dr. Michael Strano  
Massachusetts Institute of Technology  
*"New Concepts in Molecular and Energy Transport within Carbon Nanotubes and Graphene: Optical Sensors, Resonant Ion Channels, and Thermopower Waves"*

### October 24, 2013

2:30pm  
150 Chevron  
Dr. Anne McCoy  
Ohio State University  
*"Spectral Signatures of Large Amplitude Vibrations: What Information is Encoded in the Intensities?"*

4:00pm

150 Chevron  
Dr. Nicola Pohl  
Indiana University  
*"Methods Development for Automated Oligosaccharide Synthesis"*

### October 31, 2013

2:30pm  
150 Chevron  
Dr. Ben Shen  
The Scripps Research Institute  
*"Natural Product Discovery, Biosynthesis, and Engineering: Impacts on Drug Discovery and Development"*

4:00pm

150 Chevron  
Dr. Michael Ward  
New York University  
*"Diversity among Similarity: Programmed Assembly of Organic Solid State Frameworks"*

### November 7, 2013

2:30pm  
150 Chevron  
Dr. Xi Chen  
University of California-Davis  
*"Chemoenzymatic Synthesis and Applications of Carbohydrates"*

4:00pm

150 Chevron  
Dr. G. Andrés Cisneros  
Wyane State University  
*"Advances in the Development of Multipolar and Density-Based Polarizable Force Fields"*

### November 12, 2013

2:30pm  
150 Chevron  
Dr. Jennifer Schomaker  
University of Wisconsin-Madison  
*"New Transformations Mediated by Coinage Metals"*

### November 14, 2013

2:30pm  
150 Chevron  
Dr. Jon Owen  
Columbia University  
*"The Coordination Chemistry of Metal Chalcogenide Nanocrystals"*

2:30pm

150 Chevron  
Dr. Vicki Wysocki  
Ohio State University  
*"TBA"*

### November 19, 2013

27<sup>th</sup> Annual Frederick Kaufman Memorial Lecture Series  
4:00pm  
150 Chevron  
Dr. Geraldine Richmond  
University of Oregon  
*"At the Water's Edge: Understanding Environmentally Important Processes at Aqueous Surfaces"*

### November 20, 2013

27<sup>th</sup> Annual  
Frederick Kaufman Memorial Lecture Series  
2:30pm  
150 Chevron  
Dr. Geraldine Richmond  
University of Oregon  
*"Line 'Em All Up: Macromolecular and Nanoparticle Assembly at Liquid Interfaces"*

### November 21, 2013

2:30pm  
150 Chevron  
Dr. Peter Griffiths  
University of Idaho  
*"Open-Path Atmospheric Monitoring by FT-IR Spectroscopy under Pastoral and Simulated Battlefield Conditions"*

### December 9, 2013

4<sup>th</sup> Annual  
Henry Frank Lecture Series  
4:00pm  
150 Chevron  
Dr. Fred Manby  
University of Bristol  
*"Embedding Quantum Chemistry in Quantum Chemistry"*

### December 11, 2013

4<sup>th</sup> Annual  
Henry Frank Lecture Series  
4:00pm  
150 Chevron  
Dr. Fred Manby  
University of Bristol  
*"Antisymmetry and Molecular Dissociation in Coupled-Cluster Theory"*

## Society for Analytical Chemists of Pittsburgh Program Bio's Continued from pages 2 & 11

### Page 2 October Meeting

#### Dr. Igor Lednev

1983. Then Dr. Lednev worked at the Institute of Chemical Physics, Russian Academy of Sciences, as a group leader. As an academic visitor, he worked in several leading laboratories around the world including the United Kingdom, Japan, Canada and Germany. In 1997, Dr. Lednev came to the US and joined Prof. Sanford Asher laboratory at the University of Pittsburgh until he accepted a faculty position at the University at Albany in 2002. Dr. Lednev research is focused on the development and application of novel laser spectroscopy for biomedical research and forensic purposes. He has secured federal funding from the National Institutes of Health, National Science Foundation, National Institute of Justice and Air Force Office of Scientific Research. Dr. Lednev served as an advisory member for the White House Subcommittee on Forensic Science. He is on editorial boards of four scientific journals including Journal of Raman Spectroscopy, the top journal in the field, and Biochimica et Biophysica Acta, a high-ranking international journal. Dr. Lednev is a recipient of the Research Innovation Award. He has co-authored over 140 publications in peer-reviewed journals, including 2009 article in Forensics Science International, which is the most downloaded and one of the most cited paper from this top journal in the field.

### Page 11 November Meeting

#### Dr. Janusz Pawliszyn

Jubilee Medal 1998 from the Chromatographic Society, U.K., the 2000 Maxxam Award from Canadian Society for Chemistry, the 2000 Varian Lecture Award from Carleton University, the Alumni Achievement Award for 2000 from Southern Illinois University, the Humboldt Research Award for 2001, 2002 COLACRO Medal, 2003 Canada Research Chair, in 2006 he has been elected to the most cited chemists by ISI, in 2008 he received A.A. Benedetti-Pichler Award from Eastern Analytical Symposium, 2008 Andrzej Waks-mundzki Medal from Polish Academy of Sciences, 2008 Manning Principal Award, 2010 Torbern Bergman Medal from the Swedish Chemical Society, 2010 Ontario Premier's Innovation Award, 2010 Marcel Golay Award, 2010 ACS Award in Separation Science and Technology, 2011 PittCon Dal Nogare Award, 2012 E.W.R. Steacie Award, 2013 CIC Environmental Research and Development Award and 2013 CIC LeSueur Memorial Award. He presently holds the University Professor, Canada Research Chair and Natural Sciences and Engineering Research Council of Canada Industrial Research Chair in New Analytical Methods and Technologies.

## Applications for Student Travel Awards Now Being Accepted

The Pittsburgh Section of the American Chemical Society has budgeted funds to help encourage undergraduate/graduate student participation in national and regional ACS meetings. The awards are intended to help defray meeting registration and travel-related expenses (lodging, transportation, per diem) for eligible students. To apply for the funds, one should simply complete the application (available on our web site at [www.pittsburghACS.org](http://www.pittsburghACS.org)) and return it by the relevant deadline to:

Pittsburgh Section ACS  
Travel Grants  
Attn: Dr. Michelle Ward  
Room 107 / Chevron Science  
Center  
219 Parkman Avenue  
Pittsburgh, PA 15260

Each year, the Pittsburgh Section of the ACS will award up to four \$500 grants to aid our undergraduate/graduate student members in presenting papers or posters at ACS Meetings. Awards will be made based on the scientific merit of the paper/poster to be presented and financial need. The deadlines for receipt of applications are 12/01/2013 (for travel to be completed by 06/30/2014 and 06/01/2014 (for travel to be completed by 12/31/2014).

Our Section is looking forward to helping increase the participation of local students in ACS conferences. If you have any questions, please do not hesitate to contact Dr. Michelle Ward, [muscat@pitt.edu](mailto:muscat@pitt.edu) or 412-624-8064.

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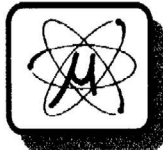
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## Services

### Volunteers Needed!

There are a number of volunteer opportunities in the Pittsburgh ACS section! If you are interested in volunteering, please contact Heather Juzwa at [hljuzwa@shimadzu.com](mailto:hljuzwa@shimadzu.com)!

### Crucible Deadline

The deadline for items submitted to The Crucible is the 1<sup>st</sup> of the month prior to publication.

For example, all items for the November 2013 issue must be to the editor by October 1, 2013.

### The Crucible

The Crucible is published monthly, August through May. Circulation, 2,500 copies per month. Subscription price, six dollars per year. All statements and opinions expressed herein are those of the editors or contributors and do not necessarily reflect the position of the Pittsburgh Section.

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## Career Opportunities

### SEARCHING FOR THAT SPECIAL JOB?

There are many companies and organizations searching for chemical and biochemical personnel to fill important jobs in their organizations.

- Companies for laboratory and management positions
- Universities & Colleges for teaching positions and laboratory personnel
- Hospitals for technical and research personnel

There are several web sites that may help you search for these open positions.

- [www.mboseervices.net/recr\\_disp.php](http://www.mboseervices.net/recr_disp.php)
- <http://pubs.acs.org/chemjobs/>

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# The Crucible

A newsletter of the Pittsburgh Section of the American Chemical Society

124 Moffett Run Rd.  
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## Change of Address

If you move, notify the American Chemical Society, 1155 Sixteenth Street, N.W., Washington, D.C. 20036.

To avoid interruption in delivery of your CRUCIBLE, please send your new address to Traci Johnsen, 124 Moffett Run Rd., Aliquippa, PA 15001. Allow two months for the change to become effective.

## Pittsburgh Area Calendar

### Monday, October 7

#### Society for Analytical Chemists of Pittsburgh

##### *"Raman Microspectroscopy and Advanced Statistics for Forensic Applications"*

Igor Lednev, Ph.D., University at Albany, State University of New York

Duquesne University, Pittsburgh, PA

### Tuesday, October 8

#### ACS Energy Technology Group

##### *"Water Management in Unconventional Gas Industry: What We Know and What We Need to Find Out"*

Professor Radisav Vidic, University of Pittsburgh  
Spaghetti Warehouse, 26<sup>th</sup> & Smallman Streets, Strip District, Pittsburgh, PA

### Tuesday, October 8

#### Greater Pittsburgh Younger Chemists Committee

##### *"Putting Your Best Foot Forward: Managing Your Paper and Online Resumes"*

University of Pittsburgh, Pittsburgh, PA

### Tuesday, October 8

#### Washington and Jefferson College Department of Chemistry Presents

##### *ACS "On The Road" Meeting, Mildred Perry Memorial Lecture*

##### *"Aqueous Electrolyte Polyionic Electrochemical Cells for Scaled Stationary Energy Storage"*

Dr. Jay Whitacre, Founder and CTO - Aquion Energy  
Washington and Jefferson College

### Saturday, October 12

#### Spectroscopy Society of Pittsburgh

##### Laboratory Tour

University of Pittsburgh, Biomedical Science Tower  
3501 Fifth Ave., Pittsburgh, PA

### Saturday, October 12

#### Spectroscopy Society of Pittsburgh

##### Continuing Education Symposium

##### Supernatural Seminar

Chevron Science Center, 219 Parkman Ave., Pittsburgh, PA

### Wednesday, October 16

#### The Spectroscopy Society of Pittsburgh

##### *"The Mars Curiosity Rover: A Year of Exploration and Evidence of Habitable Environments Beyond Earth"*

Professor Ralph Milliken, Brown University  
Duquesne University - Bayer Learning Center (Wolfe Lecture Hall), Pittsburgh, PA

### Wednesday, October 16

#### The Spectroscopy Society of Pittsburgh

##### Technology Forum

##### *"Potentially Hazardous Objects: Earth's Great Equalizer"*

Robert Marshall, Program Development Coordinator, Buhl Planetarium & Observatory at Carnegie Science Center  
Duquesne University, Pittsburgh, PA

### Friday, October 25 & Saturday, October 26

#### National Chemistry Week Event

##### *"Energy: Now and Forever"*

Carnegie Science Center, Pittsburgh, PA

### Monday, November 4

#### Society for Analytical Chemists of Pittsburgh

##### *"In-Vivo Solid Phase Microextraction"*

Janusz Pawliszyn, Ph.D., Department of Chemistry, University of Waterloo

Duquesne University, Pittsburgh, PA